

Refined comparison theorems for the Dirac equation with spin and pseudo-spin symmetry in d dimensions.

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The classic comparison theorem of quantum mechanics states that if two potentials are ordered then the corresponding energy eigenvalues are similarly ordered, that is to say if $V_a \leq V_b$, then $E_a \leq E_b$. Such theorems have recently been established for relativistic problems even though the discrete spectra are not easily characterized variationally. In this paper we improve on the basic comparison theorem for the Dirac equation with spin and pseudo-spin symmetry in $d \geq 1$ dimensions. The graphs of two comparison potentials may now cross each other in a prescribed manner implying that the energy values are still ordered. The refined comparison theorems are valid for the ground state in one dimension and for the bottom of an angular momentum subspace in $d > 1$ dimensions. For instance in a simplest case in one dimension, the condition $V_a \leq V_b$ is replaced by $U_a \leq U_b$, where $U_i(x) = \int_0^x V_i(t)dt$, $x \in [0, \infty)$, and $i = a$ or b .

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I. INTRODUCTION

Spin and pseudo-spin symmetry were first introduced in [1, 2] more than forty years ago. Spin symmetry occurs in the spectrum of a meson [3–6]. Pseudo-spin symmetry helps explain the spectra of deformed nuclei [7] and superdeformation [8], which occurs in the spectra of certain nuclei [9]. Spin symmetry helps in the design of nuclear shell-model schemes [10–12], and is used to explain certain identical bands [13–15]. Exact spin symmetry in the Dirac equation occurs when the difference between the scalar S and vector V potentials is equal to a constant, i. e. $S - V = c_1$ [4]. While exact pseudo-spin symmetry exists when the sum of scalar S and vector V potentials is equal to a constant, i. e. $S + V = c_2$ [16, 17]. Here we consider potentials of equal magnitude, so that $|S| = |V|$, and the constants c_1 and c_2 are zero.

Under spin or pseudo-spin symmetries a relativistic system of Dirac coupled equations can be written as a single Schrödinger-like equation. Then one can use methods which were developed to solve non-relativistic equations exactly or approximately, such as factorization and path-integral methods [18–22], the Nikiforov–Uvarov method [23], shape invariance [24, 25], asymptotic iteration method [26–30], supersymmetric quantum mechanics [31], and so on. For instance, the Dirac equation was solved for the Morse potential [32–36], the harmonic-oscillator potential [37–39], the pseudoharmonic potential [40], the Pöschl–Teller potential [41–44], the Woods–Saxon potential [45, 46], the Eckart potential [47, 48], the Coulomb and the Hartmann potentials [49], the Hyperbolic potentials and the Coulomb tensor interaction [50, 51], the Rosen–Morse potential [52], the Hulthén potential [53–55], the Hulthén potential including the Coulomb-like tensor potential [56], the $v_0 \tanh^2(r/d)$ potential [57], the Coulomb-like tensor potential [58], the modified Hylleraas potential [59], the Manning–Rosen and the generalized Manning–Rosen potentials [60–64], and others. The point is that there are many known exact solutions that can be used for comparisons with new potentials found in given problems.

The comparison theorem of quantum mechanics states that if the comparison potentials are ordered then the corresponding energy eigenvalues are ordered as well, i. e. if $V_a \leq V_b$ then $E_a \leq E_b$ [65–71], thus the graphs of the comparison potentials are not allowed to cross over each other. The comparison theorem was also established for

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the Dirac equation under the spin and pseudo-spin symmetry [72]. Similarly to the non-relativistic case [73], here we refine the comparison theorem for the Dirac equation under the spin and pseudo-spin symmetry by establishing conditions under which the potentials can intersect and still preserve the ordering of eigenvalues. In the simplest one-dimensional case, the condition $V_a \leq V_b$ is replaced by $U_a \leq U_b$, where $U_i(x) = \int_0^x V_i(t)dt$, $x \in [0, \infty)$, and $i = a$ or b .

The paper is organized in the following way: we start with the Dirac equation in one dimension and derive the usual comparison theorem (section II. A.). Then in section II. B. we establish some general relations between the potential V , the energy E , and mass of the particle m . In section II. C. we refine the comparison theorem, using necessary monotone behaviour of the wave functions. Finally, we demonstrate how to apply the refined comparison theorems in practice, often by taking advantage of the corollaries with specially designed simplified sufficient conditions (section II. D.). Following a similar path we then consider the family of $d > 1$ dimensional cases. In order to simplify the statements and proofs of the theorems, we shall usually combine the formulation of the spin-symmetric and pseudo-spin-symmetric cases by the use of a parameter $s = \pm 1$.

II. THE ONE-DIMENSIONAL CASE $d = 1$.

A. The Dirac equation

The Dirac equation in one dimension is given by [74]:

$$\left(\sigma_1 \frac{\partial}{\partial x} - (E - V)\sigma_3 + m + S \right) \psi = 0,$$

in natural units $\hbar = c = 1$, m is the mass of the particle, and σ_1 and σ_3 are Pauli matrices. The potentials V and S are monotone even functions such that the energy eigenvalue E exists. Both potentials are bounded at the origin, that is to say $V(0)$ and $S(0)$ are finite. By taking the two-component Dirac spinor as $\psi = \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}$ the above matrix equation can be decomposed into the following system of first-order linear differential equations [75, 76]:

$$\begin{cases} \varphi_1' = -(E + m - V + S)\varphi_2, \\ \varphi_2' = (E - m - V - S)\varphi_1, \end{cases} \quad \begin{matrix} (1a) \\ (1b) \end{matrix}$$

where the prime $'$ denotes the derivative with respect to x . For bound states, φ_1 and φ_2 satisfy the normalization condition

$$(\varphi_1, \varphi_1) + (\varphi_2, \varphi_2) = \int_{-\infty}^{\infty} (\varphi_1^2 + \varphi_2^2) dx = 1.$$

We now compare two problems with potentials V_i and S_i , $i = a$ or b , and corresponding energies E_a and E_b for which the system (1a)–(1b) becomes respectively

$$\begin{cases} \varphi_{1a}' = -(E_a + m - V_a + S_a)\varphi_{2a}, \\ \varphi_{2a}' = (E_a - m - V_a - S_a)\varphi_{1a}, \end{cases} \quad \begin{matrix} (2a) \\ (2b) \end{matrix}$$

and

$$\begin{cases} \varphi_{1b}' = -(E_b + m - V_b + S_b)\varphi_{2b}, \\ \varphi_{2b}' = (E_b - m - V_b - S_b)\varphi_{1b}. \end{cases} \quad \begin{matrix} (3a) \\ (3b) \end{matrix}$$

Let us consider the following combination of the above equations:

$$(2a)\varphi_{2b} - (2b)\varphi_{1b} - (3a)\varphi_{2a} + (3b)\varphi_{1a},$$

which, after some simplifications, becomes

$$(\varphi_{1a}\varphi_{2b})' - (\varphi_{2a}\varphi_{1b})' = (\varphi_{1a}\varphi_{1b} + \varphi_{2a}\varphi_{2b})(E_b - E_a - V_b + V_a) - (\varphi_{1a}\varphi_{1b} - \varphi_{2a}\varphi_{2b})(S_b - S_a).$$

Integrating the left side of the above expression by parts from 0 to ∞ , and using the boundary conditions, we find $\int_0^\infty [(\varphi_{1a}\varphi_{2b})' - (\varphi_{2a}\varphi_{1b})'] dx = 0$. We then integrate the right side to obtain

$$(E_b - E_a) \int_0^\infty (\varphi_{1a}\varphi_{1b} + \varphi_{2a}\varphi_{2b}) dx = \int_0^\infty [(S_b + V_b - S_a - V_a)\varphi_{1a}\varphi_{1b} + (S_a - V_a - S_b + V_b)\varphi_{2a}\varphi_{2b}] dx. \quad (4)$$

We can merge the spin and pseudo-spin symmetric cases (as was done in [72]) by introducing the parameter s , which is equal to 1 if $S = V$ and -1 if $S = -V$, so $S = sV$. Then the above expression becomes

$$(E_b - E_a) \int_0^\infty (\varphi_{1a}\varphi_{1b} + \varphi_{2a}\varphi_{2b}) dx = 2 \int_0^\infty (V_b - V_a) \varphi_{qa}\varphi_{qb} dx, \quad (5)$$

where $q = 1$ if $s = 1$ and $q = 2$ if $s = -1$. Expression (5) yields spectral ordering if the comparison potentials are ordered and the integrands have constant signs, i.e. $E_a \leq E_b$ if $V_a \leq V_b$. This is equivalent to the comparison theorem [72] which was derived by Hall and Yeşiltaş using monotonicity properties and is valid also for excited states. However, the potentials are not allowed to crossover. In the present paper we refine this theorem by letting the potentials intersect each other in a suitable controlled manner and still imply spectral ordering.

B. Classes of potentials

By differentiation and substitution, system (1a)–(1b) in the case $S = sV$ can be written as a Schrödinger-like equation

$$-\varphi'' + 2V(E + sm)\varphi = (E^2 - m^2)\varphi, \quad (6)$$

where $\varphi = \varphi_1$ if $s = 1$ and $\varphi = \varphi_2$ if $s = -1$. The radial function φ is normalizable but not necessarily normalized. In any case, and the above eigenequation determines, the eigenvalue E . By using the spectral properties of the Schrödinger operator [77], we propose to consider two subclasses of potentials: (i) V is finite for large $|x|$ and without loss of generality we choose the energy scale so that $\lim_{|x| \rightarrow \infty} V = 0$; and (ii) V is unbounded for large $|x|$ and without loss of generality we choose a coordinate system so that $V(0) = 0$. Analysing (6) and (1a)–(1b) for the $S = sV$ case we can finally state the three classes of potentials and corresponding relationship between energy E and mass m :

(i) V is finite near infinity, $sV(0) < 0$, and

$$(1) \ sV \leq 0 \text{ and } \lim_{|x| \rightarrow \infty} V = 0. \text{ This implies } -m < E < m;$$

(ii) V is unbounded near infinity, $V(0) = 0$, and

$$(2) \ sV \geq 0 \text{ and } \lim_{|x| \rightarrow \infty} V = s\infty. \text{ This implies } sE > m$$

or

$$(3) \ sV \leq 0 \text{ and } \lim_{|x| \rightarrow \infty} V = -s\infty. \text{ This implies } sE < -m.$$

For instance, consider $s = -1$ case. Then it follows from (6) that if $V \leq 0$ and $E - m > 0$ then $E^2 - m^2 < 0$. Inequality $E - m > 0$ leads to $E > m > 0$, but $E^2 - m^2 < 0$ leads to $E < -m < 0$, which is a contradiction. Then if $V \leq 0$ and $E - m < 0$ we should have $E^2 - m^2 > 0$. Both inequalities $E - m < 0$ and $E^2 - m^2 > 0$ lead to $E < -m$.

Now we assume that $\lim_{x \rightarrow \infty} V = 0$, then system (1a)–(1b) asymptotically becomes

$$\begin{cases} \varphi_1' = -(E + m)\varphi_2, \\ \varphi_2' = (E - m)\varphi_1. \end{cases} \quad (7a)$$

$$\quad (7b)$$

If $\varphi_1 \geq 0$ before vanishing, then $\varphi_1' \leq 0$ and, using $E < -m$, above system yields $\varphi_2 \leq 0$ and $\varphi_2' \leq 0$ near infinity, which is the contradiction. Assumption $\lim_{x \rightarrow \infty} V = -\infty$ leads to

$$\begin{cases} \varphi_1' = 2V\varphi_2, \\ \varphi_2' = (E - m)\varphi_1. \end{cases} \quad (8a)$$

$$\quad (8b)$$

Now if $\varphi_1 \geq 0$ and $\varphi'_1 \leq 0$ we have $\varphi_2 \geq 0$ and $\varphi'_2 \leq 0$, which means that φ_2 approaches zero with positive sign. Finally we conclude that if $S = -V$ and $V \leq 0$ then $E < -m$ and $\lim_{x \rightarrow \infty} V = -\infty$, which corresponds to (2). Following the same path, the case $s = 1$ and the remaining classes of potential and corresponding inequalities can be established.

C. Refined comparison theorems

Suppose that $\{\varphi_1(x), \varphi_2(x)\}$ is a solution of the Dirac coupled equations (1a)–(1b). Since the potential V is an even function, it follows from (1a)–(1b) that $\{\varphi_1(-x), -\varphi_2(-x)\}$ and $\{-\varphi_1(-x), \varphi_2(-x)\}$ are also solutions of (1a)–(1b). Thus φ_1 and φ_2 have definite and opposite parities, i. e. if φ_1 is even then φ_2 is odd and *vice versa*. Therefore, because of the symmetry of the wave functions, we shall consider only the positive half axis $x \geq 0$.

Now we prove the lemma which characterizes the behaviour of the one dimensional Dirac wave functions in the ground state:

Lemma 1: *In the ground state the upper φ_1 and lower φ_2 components of the Dirac spinor are monotone in the spin and pseudo-spin symmetric cases respectively.*

Proof: In the $s = -1$ case equation (1b) becomes

$$\varphi'_2 = (E - m)\varphi_1. \quad (9)$$

Since in the ground state φ_1 has constant sign, the function φ'_2 has constant sign as well, which result ends the proof. The case $s = 1$, for which the roles of φ_1 and φ_2 are interchanged, can be similarly proved. \square

For example, consider the $s = -1$ case with potential V satisfying (2). We are looking for the ground state. Thus without loss of generality, we put $\varphi_1 \geq 0$ on $[0, \infty)$. Then equation (9) yields $\varphi'_2 \leq 0$, so φ_2 has to be even and nonnegative. Consequently φ_1 is odd, so φ'_1 must change its sign from positive to negative. In order to guarantee such behaviour of φ_1 , the potential V has to be smaller than $E + m$ near the origin and then dominate the term $E + m$ at infinity: this is true since $V(0) = 0$ and $\lim_{|x| \rightarrow \infty} V = -\infty$.

Now we refine the basic comparison theorem which follows from relation (5).

Theorem 1: *The potential V belongs to one of the classes (1)–(3) and has area, $S = sV$, and*

$$g(x) = \int_0^x (V_b(t) - V_a(t))dt, \quad x \in [0, \infty). \quad (10)$$

Then if $g \geq 0$, the eigenvalues are ordered, i. e. $E_a \leq E_b$.

Proof: We prove the theorem for the pseudo-spin symmetric case, i. e. $s = -1$; for the other case the proof is essentially the same. We integrate the right side of (5) by parts to obtain

$$2 \int_0^\infty (V_b - V_a) \varphi_{2a} \varphi_{2b} dx = \varphi_{2a} \varphi_{2b} g|_0^\infty - 2 \int_0^\infty g (\varphi_{2a} \varphi_{2b})' dx,$$

where g is defined by (10). Since $g(0) = 0$ and $\lim_{x \rightarrow \infty} \varphi_2 = 0$, relation (5) becomes

$$(E_b - E_a) \int_0^\infty (\varphi_{1a} \varphi_{1b} + \varphi_{2a} \varphi_{2b}) dx = -2 \int_0^\infty g (\varphi_{2a} \varphi_{2b})' dx,$$

According to Lemma 1, φ_2 is monotone and, since it is also square integrable, it follows that the functions φ_2 and φ'_2 have different signs in the ground state, i. e. if $\varphi_2 \geq 0$ then $\varphi'_2 \leq 0$ on $[0, \infty)$ and *vice versa*. Thus the derivative of the product satisfies $(\varphi_{2a} \varphi_{2b})' \leq 0$. Finally, if $g \geq 0$, it follows from the above expression that $E_a \leq E_b$. \square

If we know more details of the interlacing relations of the comparison potentials, we can state a corollary of the above theorem which is easier to apply on practice:

Corollary 1: *Let the comparison potentials belong to one of the classes (1)–(3). If the potentials cross over once, say at x_1 , $V_a \leq V_b$ for $x \in [0, x_1]$, and*

$$g(\infty) = \int_0^\infty (V_b - V_a) dx,$$

or if the potentials cross over twice, say at x_1 and x_2 , $x_1 < x_2$, $V_a \leq V_b$ for $x \in [0, x_1]$, and

$$g(x_2) = \int_0^{x_2} (V_b - V_a) dx.$$

Then if $g(\infty) \geq 0$ and $g(x_2) \geq 0$ it follows that $g(x) \geq 0$ and the eigenvalues are ordered, i. e. $E_a \leq E_b$.

We can extend Corollary 1 to the case of n intersections, $n = 1, 2, 3, \dots$, say at points x_1, x_2, x_3, \dots . As before we suppose that $V_a \leq V_b$ on the first interval $x \in [0, x_1]$. Then we assume that the sequence $\int_{x_i}^{x_{i+1}} |V_b - V_a| dx$, $i = 1, 2, 3, \dots, n$, of absolute areas is nonincreasing (if n is odd then $\int_{x_{n-1}}^{x_n} |V_b - V_a| dx \geq \int_{x_n}^{\infty} |V_b - V_a| dx$), this leads to $g \geq 0$ on $x \in [0, \infty)$ thus, according to the first theorem, $E_a \leq E_b$.

Now we state and give proof of the second refined comparison theorem. Where the difference $V_b - V_a$ is multiplied by upper φ_1 or lower φ_2 component of the Dirac spinor.

Theorem 2: The potential V belongs to one of the classes (1)–(3) and has φ_l -weighted area, $S = sV$, and

$$p(x) = \int_0^x (V_b(t) - V_a(t)) |\varphi_l(t)| dt, \quad x \in [0, \infty). \quad (11)$$

Then if $p \geq 0$, the eigenvalues are ordered, i. e. $E_a \leq E_b$, where $\varphi_l = \varphi_{1i}$ if $s = 1$ and $\varphi_l = \varphi_{2i}$ if $s = -1$, $i = a$ or b .

Proof: We prove the theorem for the spin symmetric case and assume that the upper component of the Dirac spinor is known, so $s = 1$ and $\varphi_l = \varphi_{1i}$; for the other case the proof is essentially the same. The right side of (5) after integration by parts becomes

$$2 \int_0^\infty (V_b - V_a) \varphi_{1a} \varphi_{1b} dx = \varphi_{1b} p|_0^\infty - 2 \int_0^\infty p (\varphi_{1b})' dx,$$

where p is defined by (11) for $\varphi_{1i} = \varphi_{1a}$. The expression $\varphi_{1b} p|_0^\infty = 0$, because $p(0) = 0$ and $\lim_{x \rightarrow \infty} \varphi_1 = 0$. Then relation (5) takes the form

$$(E_b - E_a) \int_0^\infty (\varphi_{1a} \varphi_{1b} + \varphi_{2a} \varphi_{2b}) dx = -2 \int_0^\infty p (\varphi_{1b})' dx.$$

Functions φ_1 and φ_1' have different signs thus $p (\varphi_{1b})' \leq 0$ and we conclude $E_a \leq E_b$, which inequality establishes the theorem. \square

The wave functions vanish at infinity, thus the potential difference might be bigger in the second theorem than in the first one and still lead to $E_a \leq E_b$. As before we can formulate simpler sufficient condition for spectral ordering if more detailed potential behaviour is known:

Corollary 2: Let the comparison potentials belong to one of the classes (1)–(3). If the potentials cross over once, say at x_1 , $V_a \leq V_b$ for $x \in [0, x_1]$, and

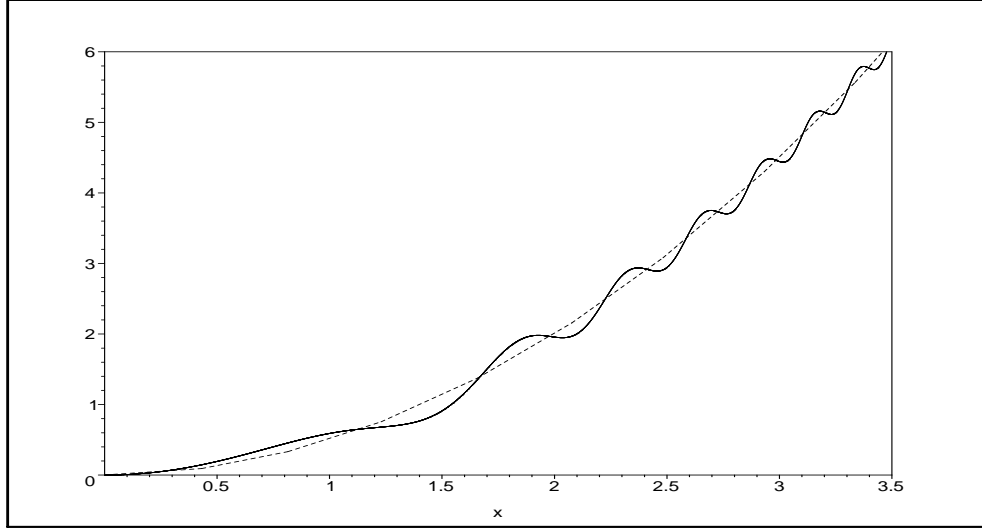
$$p(\infty) = \int_0^\infty (V_b - V_a) |\varphi_l| dx,$$

or if the potentials cross over twice, say at x_1 and x_2 , $x_1 < x_2$, $V_a \leq V_b$ for $x \in [0, x_1]$, and

$$p(x_2) = \int_0^{x_2} (V_b - V_a) |\varphi_l| dx.$$

Then if $p(\infty) \geq 0$ or $p(x_2) \geq 0$ it follows that $p(x) \geq 0$ and the eigenvalues are ordered, i. e. $E_a \leq E_b$, where $\varphi_l = \varphi_{1i}$ if $s = 1$ and $\varphi_l = \varphi_{2i}$ if $s = -1$, $i = a$ or b .

Corollary 2 can also be generalized for the case of n intersections: if $V_a \leq V_b$ on $x \in [0, x_1]$ and the sequence $\int_{x_i}^{x_{i+1}} |(V_b - V_a) \varphi_l| dx$, $i = 1, 2, 3, \dots, n$ and $\varphi_l = \varphi_{1i}$ if $s = 1$ and $\varphi_l = \varphi_{2i}$ if $s = -1$, $i = a$ or b , is nonincreasing (and, if n is odd, $\int_{x_{n-1}}^{x_n} |(V_b - V_a) \varphi_l| dx \geq \int_{x_n}^\infty |(V_b - V_a) \varphi_l| dx$), then $p \geq 0$ on $x \in [0, \infty)$, so, according to Theorem 2, we conclude $E_a \leq E_b$.


 FIG. 1: Potential V_a dashed lines and V_b full line.

D. An Example

In this section as an example we consider the extension of Corollary 1 to the case of n intersections in the spin symmetric case. We take the harmonic oscillator V_a and a modified harmonic oscillator V_b as our comparison potentials:

$$V_a = ax^2 \quad \text{and} \quad V_b = bx^2 \left(1 + \frac{\sin(x^3 + \beta)}{x^3 + \beta} \right).$$

Both comparison potentials satisfy (2) for $s = 1$. If $a = b$ the substitution $z = x^3 + \beta$ transforms the integral (10) into

$$\int_0^\infty (V_b - V_a) dt = \frac{b}{3} \int_\beta^\infty \frac{\sin z}{z} dz.$$

Choosing $\beta = 1.64$, and calculating numerical values, we find that the first area is bigger then the second one:

$$\int_\beta^\pi \frac{|\sin z|}{z} dz = 0.43810 > \int_\pi^{2\pi} \frac{|\sin z|}{z} dz = 0.43379.$$

The $\sin z$ is a periodic function, thus $|\sin x| = |\sin y|$ where $x \in [(k-1)\pi, k\pi]$ and $y = x + \pi$, $k = 3, 4, 5, \dots$, then it is clear that

$$\int_{(k-1)\pi}^{k\pi} \frac{|\sin z|}{z} dz > \int_{k\pi}^{(k+1)\pi} \frac{|\sin z|}{z} dz.$$

Therefore

$$\int_0^\infty (V_b - V_a) dt \geq 0,$$

because successive positive and negative areas of the integrand do not increase in absolute value. Thus $g > 0$ and by Theorem 1 we have $E_a \leq E_b$. This prediction is verified by accurate numerical calculations: for $a = b = 0.5$, $\beta = 1.64$, and $m = 1.2$ the comparison potentials intersect at infinitely many points (see Figure 1) and numerical eigenvalues are $E_a = 1.77935 \leq E_b = 1.85470$.

III. THE d -DIMENSIONAL CASE

A. The Dirac equation in d dimensions

The Dirac equation in $d > 1$ dimensions is given by [78]

$$i \frac{\partial \Psi}{\partial t} = H \Psi, \quad \text{where} \quad H = \sum_{s=1}^d \alpha_s p_s + (m + S)\beta + V,$$

where we use natural units $\hbar = c = 1$, m is the mass of the particle, the functions V and S are spherically symmetric vector and scalar potentials, and $\{\alpha_s\}$ and β are Dirac matrices, which satisfy anti-commutation relations; the identity matrix is implied after the potential V . The above equation can be written as the following system of two first-order differential equations [78–81]

$$\begin{cases} \psi_1' = (m + E + S - V)\psi_2 - \frac{k_d}{r}\psi_1, \\ \psi_2' = (m - E + S + V)\psi_1 + \frac{k_d}{r}\psi_2, \end{cases} \quad (12a)$$

$$\begin{cases} \psi_1' = (m + E + S - V)\psi_2 - \frac{k_d}{r}\psi_1, \\ \psi_2' = (m - E + S + V)\psi_1 + \frac{k_d}{r}\psi_2, \end{cases} \quad (12b)$$

where ψ_1 and ψ_2 are radial wave functions, $r = \|\mathbf{r}\|$, prime $'$ denotes the derivative with respect to r , $k_d = \tau(j + \frac{d-2}{2})$, $\tau = \pm 1$, and $j = 1/2, 3/2, 5/2, \dots$. We assume that the potentials V and S are such that there is an energy eigenvalue E and that equations (12a)–(12b) are the eigenequations for the corresponding pair of radial eigenstates. For $d > 1$, the wave functions vanish at $r = 0$, and for bound states they obey the normalization condition

$$(\psi_1, \psi_1) + (\psi_2, \psi_2) = \int_0^\infty (\psi_1^2 + \psi_2^2) dr = 1.$$

As in one dimension, we now compare the system (12a)–(12b) for the eigenvalues respectively E_a and E_b :

$$\begin{cases} \psi_1' = (m + E_a + S_a - V_a)\psi_{2a} - \frac{k_d}{r}\psi_{1a}, \\ \psi_2' = (m - E_a + S_a + V_a)\psi_{1a} + \frac{k_d}{r}\psi_{2a}, \end{cases} \quad (13a)$$

$$\begin{cases} \psi_1' = (m + E_a + S_a - V_a)\psi_{2a} - \frac{k_d}{r}\psi_{1a}, \\ \psi_2' = (m - E_a + S_a + V_a)\psi_{1a} + \frac{k_d}{r}\psi_{2a}, \end{cases} \quad (13b)$$

and

$$\begin{cases} \psi_1' = (m + E_b + S_b - V_b)\psi_{2b} - \frac{k_d}{r}\psi_{1b}, \\ \psi_2' = (m - E_b + S_b + V_b)\psi_{1b} + \frac{k_d}{r}\psi_{2b}. \end{cases} \quad (14a)$$

$$\begin{cases} \psi_1' = (m + E_b + S_b - V_b)\psi_{2b} - \frac{k_d}{r}\psi_{1b}, \\ \psi_2' = (m - E_b + S_b + V_b)\psi_{1b} + \frac{k_d}{r}\psi_{2b}. \end{cases} \quad (14b)$$

Then we form the following combination of the equations: $(13a)\psi_{2b} - (13b)\psi_{1b} - (14a)\psi_{2a} + (14b)\psi_{1a}$, which, after integration and some simplifications, takes the form

$$(E_b - E_a) \int_0^\infty (\psi_{1a}\psi_{1b} + \psi_{2a}\psi_{2b}) dr = \int_0^\infty [(V_b - V_a - S_a + S_b)\psi_{1a}\psi_{1b} + (V_b - V_a + S_a - S_b)\psi_{2a}\psi_{2b}] dr. \quad (15)$$

By introducing the parameter s , we can combine the spin and pseudo-spin symmetric cases, i. e. $S = sV$ where $s = 1$ if $S = V$ and $s = -1$ if $S = -V$. Then the above expression for the $S = sV$ case becomes

$$(E_b - E_a) \int_0^\infty (\psi_{1a}\psi_{1b} + \psi_{2a}\psi_{2b}) dr = 2 \int_0^\infty (V_b - V_a) \psi_{qa} \psi_{qb} dr, \quad (16)$$

where $q = 1$ if $s = 1$ and $q = 2$ if $s = -1$. If the wave functions are nodeless, i. e. have constant sign on $[0, \infty)$, and the potentials are ordered, say $V_a \leq V_b$, then the integrands of (16) have constant sign and $E_a \leq E_b$, which is equivalent to the usual comparison theorem. We shall refine that theorem later, as in the one-dimensional case. For example, we may replace $V_a \leq V_b$ by the weaker condition $\int_0^r V_b(t) t^{-2sk_a} dt \geq \int_0^r V_a(t) t^{-2sk_a} dt$ for some cases. We shall consider theorems for specific classes of potentials in section C. below.

Now, if two comparison scalar potentials S_a and S_b are equal but the vector potentials V_a and V_b are different, i. e. $S_a = S_b$ and $V_a \neq V_b$, the relation (15) can be rewritten as

$$(E_b - E_a) \int_0^\infty (\psi_{1a}\psi_{1b} + \psi_{2a}\psi_{2b})dr = \int_0^\infty (V_b - V_a)(\psi_{1a}\psi_{1b} + \psi_{2a}\psi_{2b})dr. \quad (17)$$

Then the following comparison theorem immediately follows:

Theorem 3: *If $S_a = S_b$ and $V_a \leq V_b$, then $E_a \leq E_b$.*

As an example we consider the Coulomb potential $S_a = S_b = -\frac{s}{r}$, with $s = 0.7$. For the vector potentials we choose the soft-core potential [82, 83] $V_a = -\frac{\alpha}{(r^q + a^q)^{1/q}}$ and sech-squared potential [84–87] $V_b = -\frac{4\beta}{(e^{br} + e^{-br})^2}$. If $\alpha = 0.8$, $a = 1.6$, $q = 3$, $\beta = 0.5$, and $b = 0.31$ the potentials are ordered $V_a \leq V_b$. Then, by Theorem 3, we conclude $E_a \leq E_b$, which is verified by accurate numerical eigenvalues $E_a = 0.77260 \leq E_b = 0.81648$ for $m = 1$, $\tau = -1$, $d = 5$, and $j = 1/2$.

We note that expression (17) is exactly the same as (11) from the recent work [88]. Therefore Theorem 3 can be refined in the same manner and corresponding corollaries can be derived *mutatis mutandis*.

We also note that one can derive similar theorem in one dimension. That is to say, we can obtain the expression $(E_b - E_a) \int_0^\infty (\varphi_{1a}\varphi_{1b} + \varphi_{2a}\varphi_{2b})dx = \int_0^\infty (V_b - V_a)(\varphi_{1a}\varphi_{1b} + \varphi_{2a}\varphi_{2b})dx$ from (4) and conclude that if $S_a = S_b$ and $V_a \leq V_b$, then $E_a \leq E_b$.

B. Classes of potentials

Here we characterize the relationship between the eigenvalue E and mass of the particle m depending on the type of the potential V . As in one dimension, equations (12a)–(12b) can be written in a Schrödinger-like form

$$-\psi'' + \left(\frac{k_d(k_d + s)}{r^2} + 2(E + sm)V \right) \psi = -(m^2 - E^2)\psi, \quad (18)$$

where $\psi = \psi_1$ if $s = 1$ and $\psi = \psi_2$ if $s = -1$. We shall consider the following three classes of potential:

(i) V is finite near infinity and

$$(1) \ sV \leq 0 \text{ and } \lim_{r \rightarrow \infty} V = 0. \text{ This implies } -m < E < m;$$

(ii) V is unbounded near infinity and

$$(2) \ sV \geq 0 \text{ and } \lim_{r \rightarrow \infty} V = s\infty. \text{ This implies } sE > m$$

or

$$(3) \ sV \leq 0 \text{ and } \lim_{r \rightarrow \infty} V = -s\infty. \text{ This implies } sE < -m.$$

Following a similar path as in one dimension, one can verify that the above classes of potentials and relations between energy E and mass m are valid for the system of the Dirac coupled equations (12a)–(12b) under spin and pseudo-spin symmetry.

C. Refined comparison theorems in d dimensions

In that section we refine relativistic comparison theorems in a way that the graphs of the potentials can crossover in a controlled manner with the preservation of spectral ordering. Our establishment of refined comparison theorems requires monotone behaviour of the wave function and consequently a constant sign of its derivative. But bound state wave functions are zero at the origin and vanish at infinity. Thus even if the wave function has constant sign, its derivative changes sign. The following lemma helps us to allow for this.

Lemma 2: *At the bottom of an angular-momentum subspace labelled by j , the functions $\psi_1 r^{k_d}$ and $\psi_2 r^{-k_d}$ are monotone in the spin and pseudo-spin symmetric cases respectively.*

Proof: In the case $s = 1$, using (12a)–(12b), we find

$$(\psi_1 r^{k_d})' = (m + E)\psi_2 r^{k_d}.$$

Clearly $(\psi_1 r^{k_d})'$ has constant sign since $m + E$ is constant and ψ_2 is either nonpositive or nonnegative. The case $s = -1$ can be proven similarly. \square

As in the one-dimensional case, we need to know some characteristics of the nodeless state of the Dirac coupled equations (12a)–(12b). For example, consider the case (1) with $s = 1$: according to the previous section, the potential $V \leq 0$, $\lim_{r \rightarrow \infty} V = 0$, and $-m < E < m$. The system (12a)–(12b) then takes the following form

$$\begin{cases} \psi_1' = (m + E)\psi_2 - \frac{k_d}{r}\psi_1, \\ \psi_2' = (m - E + 2V)\psi_1 + \frac{k_d}{r}\psi_2. \end{cases} \quad (19a)$$

$$\quad (19b)$$

Asymptotically near infinity the above equations become,

$$\begin{cases} \psi_1' = (m + E)\psi_2, \\ \psi_2' = (m - E)\psi_1. \end{cases} \quad (20a)$$

$$\quad (20b)$$

The components ψ_1 and ψ_2 of the Dirac spinor vanish at infinity. Suppose that $\psi_1 \geq 0$ before vanishing, then $\psi_1' \leq 0$ and it follows from the system above that $\psi_2 \leq 0$ and $\psi_2' \geq 0$. The assumption $\psi_1 \leq 0$ before vanishing, leads to $\psi_2 \geq 0$ and $\psi_2' \leq 0$. Consequently ψ_1 and ψ_2 must vanish with different signs.

Near the origin if $k_d > 0$, we set $\psi_1 \geq 0$ so $\psi_1' \geq 0$, then equation (19a) leads to $\psi_2 \geq 0$. The assumption $\psi_1 \leq 0$ would give $\psi_2 \leq 0$. The quantity $m - E + 2V$ has to change sign to guarantee the necessary behaviour of ψ_2 , i.e. increasing then decreasing if it is nonnegative or decreasing then increasing if it is nonpositive. Since $\lim_{r \rightarrow \infty} V = 0$, then $\lim_{r \rightarrow \infty} (m - E + 2V) = m - E > 0$, so $\lim_{r \rightarrow 0^+} (m - E + 2V) < 0$, thus $m - E + 2V$ changes sign exactly once from negative to positive (more details can be found in [89]). Then for $k_d < 0$ equation (19b) leads to $\psi_1 \leq 0$ if $\psi_2 \geq 0$ and *vice versa*. Hence, if $k_d > 0$ both wave function components start at the origin with the same sign, but at infinity they must have different signs: thus one of the wave function components will have at least one node in the lowest state (Figure 2, left graph). When $k_d < 0$, ψ_1 and ψ_2 start with different signs and then vanish with different signs: thus neither of them has a node in the ground state (Figure 2, right graph). Similarly analysing the case $s = -1$ and other types of potential, we get that ψ_1 and ψ_2 have no nodes if $k_d > 0$. Finally, we infer: *the Dirac radial wave functions ψ_1 and ψ_2 , which satisfy (12a)–(12b), are node free in the case $S = sV$ if $sk_d < 0$.* We note that Alberto *et. al.* in the recent work [93] derived general result: $n_1 = n_2$ if $sk_d < 0$, where n_1 and n_2 are the numbers of nodes of ψ_1 and ψ_2 respectively. Now, using this result, we state and prove the refined comparison theorem.

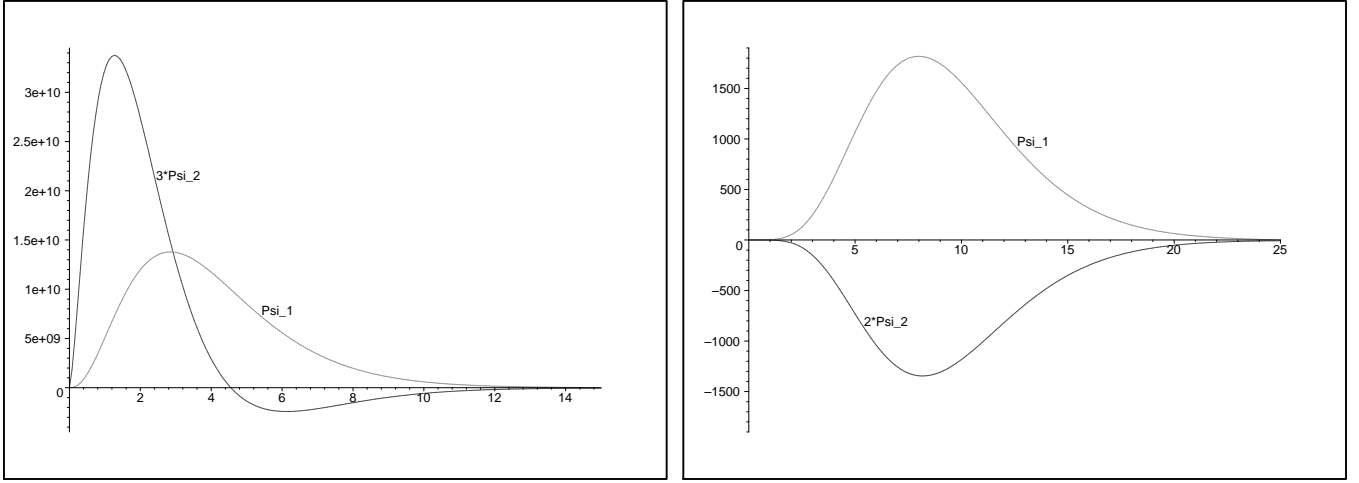


FIG. 2: Ground state of the Dirac coupled equations (12a)–(12b) in the spin-symmetric case, $V = S$, for the cut-off Coulomb potential [90–92] $V = -\frac{v}{r+a}$. Left graph: $\tau = 1$, $m = 1$, $d = 4$, $j = 1/2$, $v = 1.5$, $a = 0.01$, and $E = 0.47399$. Right graph: $\tau = -1$, $m = 1$, $d = 7$, $j = 5/2$, $v = 2.5$, $a = 1.2$, and $E = 0.69329$.

Theorem 4: *The potential V belongs to one of the classes (1)–(3) and has r^{-2sk_d} -weighted area, $S = sV$, $sk_d < 0$, and*

$$\rho(r) = \int_0^r (V_b(t) - V_a(t))t^{-2sk_d} dt, \quad r \in [0, \infty). \quad (21)$$

Then if $\rho \geq 0$, the eigenvalues are ordered, i. e. $E_a \leq E_b$.

Proof: We prove the theorem for the spin symmetric case, i. e. $s = 1$; for the other case the proof is similar. Let us integrate by parts the right side of (16) in the following way

$$\int_0^\infty (V_b - V_a)\psi_{1a}\psi_{1b}dr = \psi_{1a}\psi_{1b}\rho r^{2k_d}\Big|_0^\infty - \int_0^\infty \rho (\psi_{1a}\psi_{1b}r^{2k_d})' dr,$$

where ρ is defined by (21). Since $\rho(0) = 0$ and $\lim_{r \rightarrow \infty} \psi_1 = 0$, relation (16) becomes

$$(E_b - E_a) \int_0^\infty (\psi_{1a}\psi_{1b} + \psi_{2a}\psi_{2b})dr = - \int_0^\infty \rho (\psi_{1a}\psi_{1b}r^{2k_d})' dr. \quad (22)$$

Since ψ_1 vanishes at infinity, the function $\psi_1 r^{k_d}$ vanishes as well. Thus, according to Lemma 2, the functions $(\psi_1 r^{k_d})'$ and $\psi_1 r^{k_d}$ have different signs, which leads to $(\psi_{1a}\psi_{1b}r^{2k_d})' \leq 0$. Then it follows from expression (22) that the nonnegativity of ρ and the nodeless form of the wave functions result in $E_a \leq E_b$. \square

As in the one-dimensional case, if we know more details concerning the behaviour of the comparison potentials, we can state simpler sufficient conditions:

Corollary 4: *Let the comparison potentials belong to one of the classes (1)–(3). If the potentials cross over once, say at r_1 , $V_a \leq V_b$ for $r \in [0, r_1]$, and*

$$\rho(\infty) = \int_0^\infty (V_b - V_a)r^{-2sk_d} dr,$$

or if the potentials cross over twice, say at r_1 and r_2 , $r_1 < r_2$, $V_a \leq V_b$ for $r \in [0, r_1]$, and

$$\rho(r_2) = \int_0^{r_2} (V_b - V_a)r^{-2sk_d} dr.$$

Then if $\rho(\infty) \geq 0$ and $g(x_2) \geq 0$ it follows that $\rho \geq 0$ and the eigenvalues are ordered, i. e. $E_a \leq E_b$.

We can extend the above corollary in the following way: assume that comparison potentials have n intersections, $n = 1, 2, 3, \dots$, and $V_a \leq V_b$ on $r \in [0, r_1]$. Also assume that $\int_{r_i}^{r_{i+1}} |V_b - V_a| r^{-2sk_d} dr$, $i = 1, 2, 3, \dots, n$ (if n is odd then $\int_{r_{n-1}}^{r_n} |V_b - V_a| r^{-2sk_d} dr \geq \int_{r_n}^{\infty} |V_b - V_a| r^{-2sk_d} dr$), hence $\rho(r) \geq 0$ for $r \in [0, \infty)$, and we conclude $E_a \leq E_b$. In the same manner we prove the following theorem:

Theorem 5: *The potential V belongs to one of the classes (1)–(3) and has $\psi_l r^{-sk_d}$ -weighted area, $S = sV$, $sk_d < 0$, and*

$$\mu(r) = \int_0^r (V_b(t) - V_a(t)) |\psi_l(t)| t^{-sk_d} dt, \quad r \in [0, \infty). \quad (23)$$

Then if $\mu \geq 0$, the eigenvalues are ordered, i. e. $E_a \leq E_b$, where $\psi_l = \psi_{1i}$ if $s = 1$ and $\psi_l = \psi_{2i}$ if $s = -1$, $i = a$ or b .

Proof: We prove the theorem for the pseudo-spin symmetric case and assume that ψ_2 lies above the r -axis i. e. $s = -1$ and $\psi_2 \geq 0$; for the other case the proof is similar. We integrate the right side of (16) to obtain

$$(E_b - E_a) \int_0^\infty (\psi_{1a}\psi_{1b} + \psi_{2a}\psi_{2b}) dr = - \int_0^\infty \mu (\psi_{2a} r^{-k_d})' dr,$$

where μ is defined by (23) for $i = b$. Since $\psi_{2a} \geq 0$, then $\psi_{2a} r^{-k_d} \geq 0$ and, according to Lemma 2, $(\psi_{2a} r^{-k_d})' \leq 0$. Thus the product $\mu (\psi_{2a} r^{-k_d})'$ is nonpositive and the above expression leads to $E_a \leq E_b$. \square

Corollary 5: *Let the comparison potentials belong to one of the classes (1)–(3). If the potentials cross over once, say at r_1 , $V_a \leq V_b$ for $r \in [0, r_1]$, and*

$$\mu(\infty) = \int_0^\infty (V_b - V_a) |\psi_l| r^{-sk_d} dr,$$

or if the potentials cross over twice, say at r_1 and r_2 , $r_1 < r_2$, $V_a \leq V_b$ for $r \in [0, r_1]$, and

$$\mu(r_2) = \int_0^{r_2} (V_b - V_a) |\psi_l| r^{-sk_d} dr.$$

Then if $\mu(\infty) \geq 0$ or $\mu(r_2) \geq 0$ it follows that $\mu(r) \geq 0$ and the eigenvalues are ordered, i. e. $E_a \leq E_b$, where $\psi_l = \psi_{1i}$ if $s = 1$ and $\psi_l = \psi_{2i}$ if $s = -1$, $i = a$ or b .

As before we can generalize Corollary 5 to allow n intersections, i.e. if $V_a \leq V_b$ on $r \in [0, r_1]$ and sequence of absolute areas $\int_{r_i}^{r_{i+1}} |(V_b - V_a) \psi_l r^{-sk_d}| dr$ is nonincreasing (if n is odd then we assume $\int_{r_{n-1}}^{r_n} |(V_b - V_a) \psi_l r^{-sk_d}| dr \geq \int_{r_n}^{\infty} |(V_b - V_a) \psi_l r^{-sk_d}| dr$), then integral $\int_0^r (V_b(t) - V_a(t)) \psi_l(t) t^{-sk_d} dt \geq 0$ for $r \in [0, \infty)$, so $E_a \leq E_b$.

D. An example

Here we will demonstrate the first part of Corollary 5, i.e. the case of one intersection. For the comparison potentials we choose the Yukawa potential [94] V_a and the Coulomb potential V_b , which satisfy (1) for $s = 1$:

$$V_a = -\frac{\alpha}{r e^{ar}} \quad \text{and} \quad V_b = -\frac{\beta}{r}.$$

The solutions of the Dirac Coulomb problem are well known; in particular, article [72] provides us with the eigenvalue equation and the ground state wave function for $d = 2$, $j = 1/2$, $\tau = -1$, and $m = 1$ in the spin-symmetric case:

$$E_b^2 - 1 = -(2\beta(E_b + 1))^2 \quad \text{and} \quad \psi_b = \sqrt{r} e^{-r\sqrt{1-E_b^2}}.$$

Fixing $\alpha = 0.2$ and $a = 0.1$ and varying $\beta = 0.172$, the above potentials intersect at exactly one point (Figure 3, left graph) so that $V_a \leq V_b$ before the intersection point. A direct numerical calculation shows

$$\mu(\infty) = \int_0^\infty (V_b - V_a) \psi_b \sqrt{r} dr = 0.00006$$

Hence, according to Corollary 5, $E_a \leq E_b$, which we have verified by an accurate calculation: $E_a = 0.75632 \leq E_b = 0.78837$. We also can obtain a lower bound for E_a using the usual comparison theorem, which follows from (16). Keeping $\alpha = 0.2$ and $a = 0.1$ and choosing $\beta = 0.201$ we have $V_a > V_b$ on $r \in [0, \infty)$ (see Figure 4, right graph). Therefore $E_a = 0.75632 > E_b = 0.70010$.

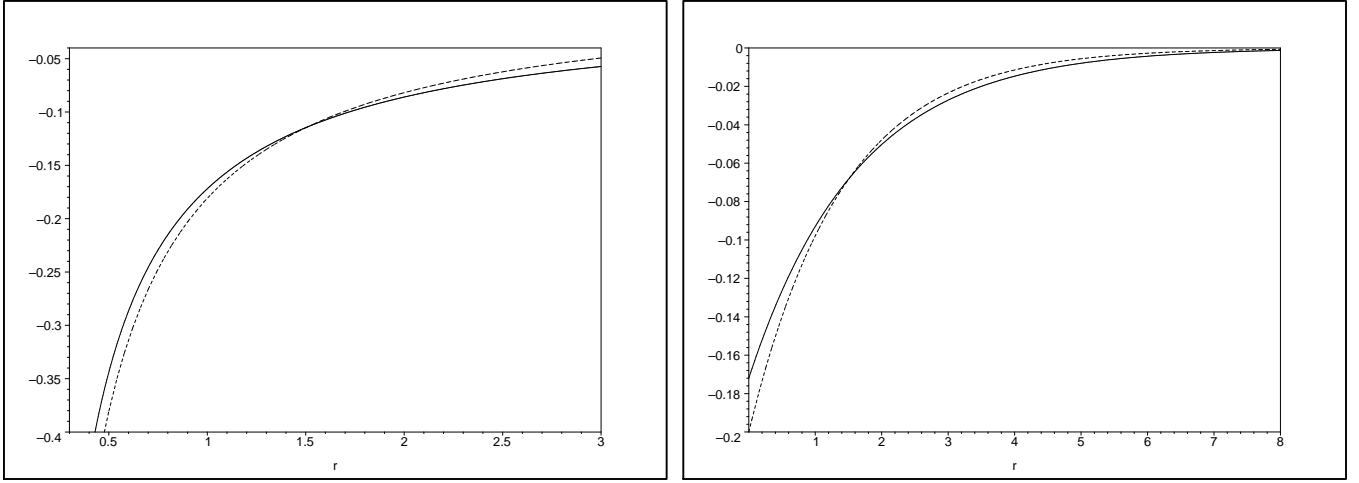


FIG. 3: Left graph: The Yukawa potential V_a (dotted line) and the Coulomb potential V_b (full line). Right graph: the functions $V_a \psi_b \sqrt{r}$ (dotted line) and $V_b \psi_b \sqrt{r}$ (full line).

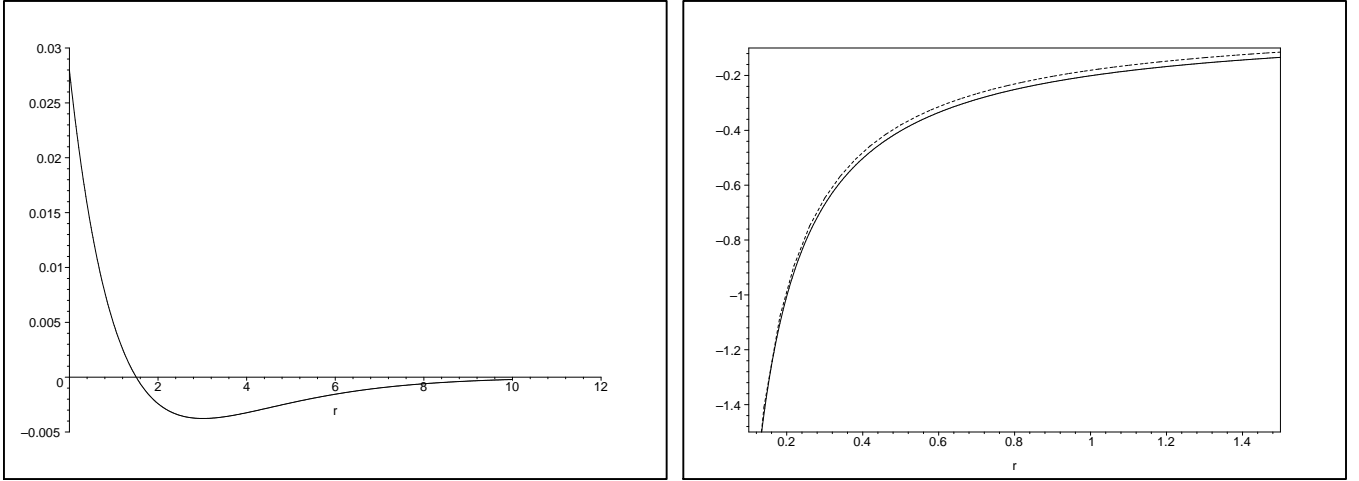


FIG. 4: Left graph: The graph of the integrand $I = (V_b - V_a) \psi_b \sqrt{r}$. Right graph: The Coulomb potential V_a (dotted line) and the Yukawa potential V_b (full line).

IV. CONCLUSION

The systems of Dirac coupled equations in one dimension (1a)–(1b) and $d > 1$ dimensions (12a)–(12b) are studied here for the spin-symmetric and pseudo-spin-symmetric cases. The treatment of these two cases has been unified by the introduction of the parameter s which takes the value $s = 1$ if $S = V$ and $s = -1$ if $S = -V$, thus $S = sV$. By writing the above systems in a Schrödinger-like form and analyzing their behaviour near the origin and at infinity, we are able to consider three appropriate and interesting classes of potential, with corresponding general relations between energy E and the mass of the particle m . The structure of the nodeless states were discussed, and certain monotone behaviours of the wave functions were established (Lemma 1 and Lemma 2). Using these results we have refined the comparison theorems for the Dirac equations in the $S = sV$ cases. In fact, the condition $V_a \leq V_b$ which leads to $E_a \leq E_b$ may now be replaced by $U_a \leq U_b$, where in each case U is a specific integral transform of V that induces a weaker condition leading to the same spectral ordering $E_a \leq E_b$. For problems where it is found to be complicated to apply these theorems immediately, corresponding corollaries have been established for the cases of one, two, and n intersections of the comparison-potential graphs. The application of these theorems is illustrated by a variety of explicit examples in one and $d > 1$ dimensions. Since, exact analytical solutions for spin-symmetric and pseudo-spin-

symmetric problems are plentiful in the literature, there is reason to expect that an approximation theory based on such comparison theorems might offer a useful tool for relativistic spectral estimation.

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